



PREDICTING THE FUNCTIONAL STATE OF PROTEIN KINASES USING INTERPRETABLE GRAPH NEURAL NETWORKS



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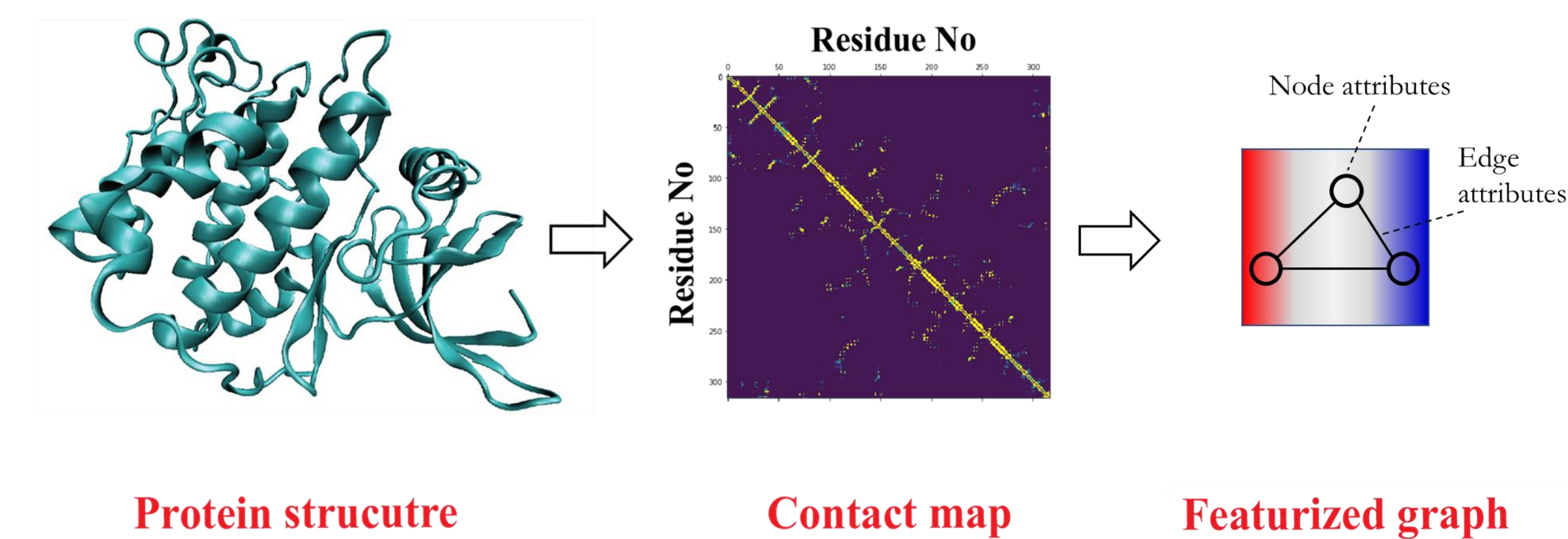
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Overview

- ❑ Protein kinases regulate several essential cellular activities, the dysfunction of which is implicated in several cancers
- ❑ Automatic identification of structurally important moieties is critical for drug discovery/design

We develop interpretable graph neural network (GNN) based deep learning framework for classifying the functionally active and inactive states of protein kinases using their 3D structures

Methods



GNN for protein classification and Gradient-weighted Class Activation Mapping (Grad-CAM) for identifying structurally important motifs

Key Takeaways

- ❑ GNN models can classify protein kinases with greater than 97% accuracy
- ❑ Grad-CAM identifies several well-known conserved regions and also other lesser-known functionally relevant moieties of the kinases
- ❑ Using the interpretable framework, the structural differences between thousands of crystal structures can be analyzed

More Information

Please visit the poster session on Tuesday (Feb 22 – 1:45 to 2:45 PM), Protein Structure and Conformation III, Board B7 for unpublished results and detailed discussions on the topic